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The Selection of a Multivariable Approximating Function Satisfying a Given Error Tolerance in the Sense of Least Squares

by

Daniel E. Dupree, F. L. Harmon, R. A. Hickman
Edward Anders and James O'Neil

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SUMMARY

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A technique for obtaining a function which yields an error, in the sense of least squares, that is less than a specified tolerance is developed.

AUTHOR

I. INTRODUCTION

In [1] , a recursion process was developed for obtaining the coefficients $A_0, A_1, \ldots, A_N$ of the function $A_0\varphi_0(\beta) + A_1\varphi_1(\beta) + - -$ $- + A_N\varphi_N(\beta)$ such that

$$E = \sum_{i=0}^{n} \left\{ X(\beta_i) - \sum_{j=0}^{N} A_j\varphi_j(\beta_i) \right\}^2$$

is minimum. This scheme yields the coefficients of the approximating function without having to solve the normal equations. Of course, the least squares procedure minimizes the sum of the squared errors, yet we have no assurance of the relative size of this error. In this report, we will develop a process for choosing the approximating function in such a fashion that the error will not exceed a given tolerance.

Before doing this, let us examine more closely the error E incurred by using the function $\sum_{j=0}^{N} A_j\varphi_j(\beta)$ as an approximating function. If the vectors $\bar{\varphi}_0, \bar{\varphi}_1, \ldots, \bar{\varphi}_N$, $N < n$, are used to obtain the collection $\bar{e}_0, \bar{e}_1, \ldots, \bar{e}_N$ of orthonormal vectors as in [1] , then the error E can be written as follows:

$$E = \sum_{i=0}^{n} \left[X(\beta_i) - \sum_{j=0}^{N} A_j\varphi_j(\beta_i) \right]^2 = \| \bar{X} - A_0\bar{\varphi}_0 - A_1\bar{\varphi}_1 -$$

$$\ldots - A_N\bar{\varphi}_N \|^2 = \| \bar{X} - \sum_{j=0}^{N} (\bar{X}, \bar{e}_j)\,\bar{e}_j \|^2 =$$

$$\| \bar{X} \|^2 - \left[\bar{X}, \sum_{j=0}^{N} (\bar{X}, \bar{e}_j)\,\bar{e}_j \right] - \left[\bar{X}, \sum_{j=0}^{N} (\bar{X}, \bar{e}_j)\,\bar{e}_j \right] +$$

$$\| \sum_{j=0}^{N} (\bar{X}, \bar{e}_j)\,\bar{e}_j \|^2 = \| \bar{X} \|^2 - \sum_{j=0}^{N} (\bar{X}, \bar{e}_j)^2 .$$

From this representation of E, we are able to observe the following:

1) $\| \overline{X} \|^2$ is an upper bound for E.

2) A sum of any k of the N + 1 terms $(\overline{X}, \overline{e}_j)^2$, $0 < k < N$, will yield an error $E' > E$.

3) If $\overline{e}_{N+1}$ is any other non-zero vector orthogonal to each of $\overline{e}_0, \overline{e}_1, \ldots, \overline{e}_N$, then $\| \overline{X} \|^2 - \sum_{j=0}^{N+1} (\overline{X}, \overline{e}_j)^2 < E$.

II. SELECTION OF THE FUNCTION

After evaluating $\| \overline{X} \|^2 - \sum_{j=0}^{N} (\overline{X}, \overline{e}_j)^2$, we may find that this value still exceeds a given error tolerance δ. Then we wish to find $\overline{\varphi}_{N+1}$ such that

$$\| \overline{X} \|^2 - \sum_{j=0}^{N} (\overline{X}, \overline{e}_j)^2 - (\overline{X}, \overline{e}_{N+1})^2 \leq \delta;$$

i.e., find $\overline{\varphi}_{N+1}$ such that

$$(\overline{X}, \overline{e}_{N+1})^2 \geq \| \overline{X} \|^2 - \sum_{j=0}^{N} (\overline{X}, \overline{e}_j)^2 - \delta,$$

where $\overline{e}_{N+1}$ is the vector associated with $\overline{\varphi}_{N+1}$ that is orthonormal to $\overline{e}_0, \overline{e}_1, \ldots, \overline{e}_N$.

Suppose we let

$$\overline{\varphi}_{N+1} = (\lambda_0, \lambda_1, \ldots, \lambda_n).$$

Then

$$\bar{\varphi}'_{N+1} = \bar{\varphi}_{N+1} - (\bar{\varphi}_{N+1}, \bar{e}_0)\, \bar{e}_0 - \dots - (\bar{\varphi}_{N+1}, \bar{e}_N)\, \bar{e}_N$$

$$= (\lambda_0, \lambda_1, \dots, \lambda_n) - \left(\sum_{i=0}^{n} \lambda_i\, e_{0i}\right) \bar{e}_0 - \dots$$

$$- \left(\sum_{i=0}^{n} \lambda_i\, e_{Ni}\right) \bar{e}_N,$$

if $\bar{e}_j = (e_{j0}, e_{j1}, \dots, e_{jn})$, $j = 0,1,\dots,N$.

Therefore,

$$\bar{e}_{N+1} = \frac{(\lambda_0,\lambda_1,\dots,\lambda_n) - \left(\sum_{i=0}^{n} \lambda_i\, e_{0i}\right) \bar{e}_0 - \dots - \left(\sum_{i=0}^{n} \lambda_i\, e_{Ni}\right) \bar{e}_N}{\left\{\sum_{i=0}^{n} \lambda_i^2 - \left(\sum_{i=0}^{n} \lambda_i\, e_{0i}\right)^2 - \dots - \left(\sum_{i=0}^{n} \lambda_i\, e_{Ni}\right)^2\right\}^{1/2}},$$

and if $\bar{X} = (t_0, t_1, \dots, t_n)$, then

$$(\bar{X}, \bar{e}_{N+1})^2 = \frac{\left[\sum_{i=0}^{n} \lambda_i\, t_i - \left(\sum_{i=0}^{n} \lambda_i\, e_{0i}\right)(\bar{X}, \bar{e}_0) - \dots - \left(\sum_{i=0}^{n} \lambda_i\, e_{Ni}\right)(\bar{X}, \bar{e}_N)\right]^2}{\sum_{i=0}^{n} \lambda_i^2 - \left(\sum_{i=0}^{n} \lambda_i\, e_{0i}\right)^2 - \dots - \left(\sum_{i=0}^{n} \lambda_i\, e_{Ni}\right)^2}.$$

Thus, to have

$$(\bar{X}, \bar{e}_{N+1})^2 \geq \|\bar{X}\|^2 - \sum_{j=0}^{N} (\bar{X}, \bar{e}_j)^2 - \delta,$$

we must have

$$\left[\sum_{i=0}^{n} \lambda_i\, t_i - \left(\sum_{i=0}^{n} \lambda_i\, e_{0i}\right)(\bar{X}, \bar{e}_0) - \dots - \left(\sum_{i=0}^{n} \lambda_i\, e_{Ni}\right)(\bar{X}, \bar{e}_N)\right]^2 \geq$$

$$\left[\sum_{i=0}^{n} \lambda_i^2 - \left(\sum_{i=0}^{n} \lambda_i\, e_{0i}\right)^2 - \dots - \left(\sum_{i=0}^{n} \lambda_i\, e_{Ni}\right)^2\right] \left[\|\bar{X}\|^2 - \sum_{j=0}^{N} (\bar{X}, \bar{e}_j)^2 - \delta\right],$$

or

$$\left[\sum_{i=0}^{n} \lambda_i \{t_i - (\overline{X}, \overline{e}_0)\, e_{0i} - \dots - (\overline{X}, \overline{e}_N)\, e_{Ni}\}\right]^2 \geq$$

$$\left[\sum_{i=0}^{n} \lambda_i^2 - \left(\sum_{i=0}^{n} \lambda_i e_{0i}\right)^2 - \dots - \left(\sum_{i=0}^{n} \lambda_i e_{Ni}\right)^2\right]\left[\|\overline{X}\|^2 - \sum_{j=0}^{N} (\overline{X}, \overline{e}_j)^2 - \delta\right],$$

or

$$\sum_{i=0}^{n} \left[\lambda_i^2 \{t_i - (\overline{X}, \overline{e}_0)\, e_{0i} - \dots - (\overline{X}, \overline{e}_N)\, e_{Ni}\}^2\right.$$

$$+ 2\lambda_i \sum_{\substack{k=0\\k>i}}^{n} \lambda_k \{t_i - (\overline{X}, \overline{e}_0)\, e_{0i} - \dots - (\overline{X}, \overline{e}_N)\, e_{Ni}\}\{t_k - (\overline{X}, \overline{e}_0)\, e_{0k} -$$

$$\left.\dots - (\overline{X}, \overline{e}_N)\, e_{Nk}\}\right] \geq \sum_{i=0}^{n} \left[\lambda_i^2 - \lambda_i^2 e_{0i}^2 - 2\lambda_i \sum_{\substack{k=0\\k>i}}^{n} \lambda_k e_{0i} e_{0k} - \dots\right.$$

$$\left. - \lambda_i^2 e_{Ni}^2 - 2\lambda_i \sum_{\substack{k=0\\k>i}}^{n} \lambda_k e_{Ni} e_{Nk}\right]\left[\|\overline{X}\|^2 - \sum_{j=0}^{N} (\overline{X}, \overline{e}_j)^2 - \delta\right],$$

or

$$\sum_{i=0}^{n} \left[\lambda_i^2 \left\{\{t_i - (\overline{X}, \overline{e}_0)\, e_{0i} - \dots - (\overline{X}, \overline{e}_N)\, e_{Ni}\}^2 - \{\|\overline{X}\|^2 - \right.\right.$$

$$\sum_{j=0}^{N} (\overline{X}, \overline{e}_j)^2 - \delta\} + e_{0i}^2 \{\|\overline{X}\|^2 - \sum_{j=0}^{N} (\overline{X}, \overline{e}_j)^2 - \delta\} + \dots +$$

$$e_{Ni}^2 \ \{ \| \overline{X} \|^2 - \sum_{j=0}^{N} (\overline{X}, \overline{e}_j)^2 - \delta\} \Big\} + \lambda_i \Big\{ 2 \sum_{\substack{k=0 \\ k>i}}^{n} \lambda_k \{t_i - (\overline{X}, \overline{e}_0) e_{0i}$$

$$- \dots - (\overline{X}, \overline{e}_N) e_{Ni}\}\{t_k - (\overline{X}, \overline{e}_0) e_{0k} - \dots - (\overline{X}, \overline{e}_N) e_{Nk}\} +$$

$$2 \{ \| \overline{X} \|^2 - \sum_{j=0}^{N} (\overline{X}, \overline{e}_j)^2 - \delta\}\{ \sum_{\substack{k=0 \\ k>i}}^{n} \lambda_k e_{0i} e_{0k} + \dots + \sum_{\substack{k=0 \\ k>i}}^{n} \lambda_k e_{Ni} e_{Nk}\} \Big\} \Big]$$

$$\geq 0.$$

If we let

$$A_i = \Big\{\{t_i - (\overline{X}, \overline{e}_0) e_{0i} - \dots - (\overline{X}, \overline{e}_N) e_{Ni}\}^2 - \{ \| \overline{X} \|^2 - \sum_{j=0}^{N} (\overline{X}, \overline{e}_j)^2 - \delta\}$$

$$+ e_{0i}^2 \ \{ \| \overline{X} \|^2 - \sum_{j=0}^{N} (\overline{X}, \overline{e}_j)^2 - \delta\} + \dots + e_{Ni}^2 \ \{ \| \overline{X} \|^2 - \sum_{j=0}^{N} (\overline{X}, \overline{e}_j)^2 - \delta\} \Big\},$$

and

$$B_i = 2 \Big\{ \sum_{\substack{k=0 \\ k>i}}^{n} \lambda_k \{t_i - (\overline{X}, \overline{e}_0) e_{0i} - \dots - (\overline{X}, \overline{e}_N) e_{Ni}\}\{t_k - (\overline{X}, \overline{e}_0) e_{0k} -$$

$$\dots - (\overline{X}, \overline{e}_N) e_{Nk}\} + \{ \| \overline{X} \|^2 - \sum_{j=0}^{N} (\overline{X}, \overline{e}_j)^2 - \delta\}\{ \sum_{\substack{k=0 \\ k>i}}^{n} \lambda_k e_{0i} e_{0k} +$$

$$\dots + \sum_{\substack{k=0 \\ k>i}}^{n} \lambda_k e_{Ni} e_{Nk}\} \Big\},$$ we can write this inequality as

$\sum_{i=0}^{n} (A_i \lambda_i^2 + B_i \lambda_i) \geq 0$, and this inequality is satisfied if

$A_i \lambda_i^2 + B_i \lambda_i \geq 0$, for $i = 0, 1, \ldots, n$. Notice that these conditions are much stronger than are necessary and we will need to examine some cases that might arise.

Case 1: If $A_i \geq 0$ for some i, $0 \leq i \leq n$, choose $\lambda_t = 0$, $t = n, n-1, \ldots, i_0 + 1$, where i_0 is the largest value of i such that $A_i \geq 0$, $\lambda_{i_0} = 1$, and $\lambda_k = -\frac{B_k}{A_k}$, $k = 0, 1, \ldots, i_0 - 1$, provided $A_k \neq 0$, or $\lambda_k = B_k$, $k = 0, 1, \ldots, i_0 - 1$, for $A_k = 0$.

Case 2: If $A_i < 0$, for all i, tentatively choose $\lambda_k = 1$ and examine

(1) $B_{k-1}^2 - 4A_k A_{k-1} \geq 0$, $k = n, n-1, \ldots, 2, 1, 0$.

If (1) is not true, choose $\lambda_k = 0$ and proceed to examine,

(2) $B_{k-2}^2 - 4A_{k-1} A_{k-2} \geq 0$ for $\lambda_{k-1} = 1$.

If (2) is false, choose $\lambda_{k-1} = 0$ and proceed as before.

If (1) is satisfied for some value of k, let i be the first such positive integer in the sequence n, n-1, ... , 1, 0. Then $(B_{i-1})^2 - 4A_{i-1} A_i \lambda_i^2 \geq 0$, and we are assured of a solution λ_{i-1} to the equation

$$A_{i-1} \lambda_{i-1}^2 + B_{i-1} \lambda_{i-1} + A_i \lambda_i^2 = 0.$$

Notice that the left side of this equation is just the sum of the ith and (i-1)st terms of the sum $\sum_{i=0}^{n} (A_i \lambda_i^2 + B_i \lambda_i)$. Thus, let λ_{i-1} be either solution of the equation

$$A_{i-1} \lambda_{i-1}^2 + B_{i-1} \lambda_{i-1} + A_i \lambda_i^2 = 0.$$

Then $\lambda_j = -\frac{B_j}{A_j}$, j = i-1, ... , 1, 0, will assure the satisfaction of the suceeding inequalities.

In the newly computed vector $\bar{\varphi}_{N+1} = (\lambda_0, \lambda_1, \ldots, \lambda_n)$, suppose we let λ_i be the value of some ideal function $\varphi_{N+1}(\beta)$ at β_i; i.e., $\varphi_{N+1}(\beta_i) = \lambda_i$. Then this ideal function assures us that the error E, where

$$E = \sum_{i=0}^{n} \left[X(\beta_i) - \sum_{j=0}^{N} A_j \varphi_j(\beta_i) - A_{N+1} \varphi_{N+1}(\beta_i) \right]^2,$$

is less than the imposed tolerance δ. Since we know the values of this ideal function at the tabular values β_i, our next objective is to develop a technique for computing $\varphi_{N+1}(\beta')$, for some value $\beta' \neq \beta_i$, $i = 0,1,\ldots,n$, such that the error obtained by using $\sum_{j=0}^{N+1} A_j\, \varphi_j(\beta')$ to approximate $X(\beta')$, in the sense of least squares, is as small, if not smaller, than the error obtained by approximating $X(\beta')$ with $\sum_{j=0}^{N} A_j\, \varphi_j(\beta')$. We obtain this value $\varphi_{N+1}(\beta')$ in the following manner.

First, we compute $A_{N+1}(k)$, $k = -1, 0, 1, \ldots, N$, $\bar{e}_{N+1}$ and A'_{N+1} as follows:

$$A_{N+1}(-1) = \frac{1}{\left\| \bar{\varphi}_{N+1} - \sum_{j=0}^{N} (\bar{\varphi}_{N+1}, \bar{e}_j)\, \bar{e}_j \right\|}$$

$$A_{N+1}(0) = A_{N+1}(-1)\, A_0(-1)(\bar{\varphi}_{N+1}, \bar{\varphi}_0)$$

$$\vdots$$

$$A_{N+1}(N) = A_{N+1}(-1)\, A_N(-1)(\bar{\varphi}_{N+1}, \bar{\varphi}_N) - \sum_{j=0}^{N-1} A_{N+1}(j)\, A_N(j).$$

$$\bar{e}_{N+1} = A_{N+1}(-1)\, \bar{\varphi}_{N+1} - \sum_{j=0}^{N} A_{N+1}(j)\, \bar{e}_j$$

$$A'_{N+1} = (\bar{X}, \bar{e}_{N+1}).$$

Finally, compute the $(N+2)$ A_j's, $j = 0, 1, \ldots, N+1$, as follows:

$$A_{N+1} = A'_{N+1}\, A_{N+1}(-1)$$

$$A_N = A_N(-1) \left[A'_N - A'_{N+1} A_{N+1}(N) \right]$$

$$A_{N-1} = A_{N-1}(-1) \left\{ A'_{N-1} - A'_N A_N(N-1) + A'_{N+1} \left[- A_{N+1}(N-1) + A_{N+1}(N) A_N(N-1) \right] \right\},$$

$$\vdots$$

Now let $\beta_{i'}$ be a β_i such that $\| \beta_{i'} - \beta' \| = \min\limits_{0 \leq i \leq n} \left\{ \| \beta_i - \beta' \| \right\}$,

and let us define the following function:

$$\sum_{j=0}^{N} A_j \varphi_j (\beta') + A_{N+1} M(\beta'),$$

$$\text{where } M(\beta') = \lambda_{i'} \left[\frac{L(\beta_{i'}) - 2 \| \beta_{i'} - \beta' \|}{L(\beta_{i'})} \right],$$

$$\text{for } 2 \| \beta_{i'} - \beta' \| < L(\beta_{i'}),$$

$$= 0, \text{ otherwise},$$

$$\text{where } L(\beta_{i'}) = \min_{\substack{0 \leq i \leq n \\ i \neq i'}} \left\{ \| \beta_i - \beta_{i'} \| \right\}.$$

Thus, when β' is chosen, we are able to use the function above to approximate $X(\beta')$, being assured that the approximation obtained here is no worse that the value $\sum_{j=0}^{N} A_j \varphi_j (\beta')$ obtained by using the initial least squares approximating function.

Writing this multiple of λ_i as

$$\frac{\frac{1}{2} L(\beta_{i'}) - \| \beta_{i'} - \beta' \|}{\frac{1}{2} L(\beta_{i'})},$$

we see that we have a factor which varies from zero to one as β' varies from a position on the boundary to a position at the center of the ball

$$\left\{ \beta \,\middle|\, \| \beta_{i'} - \beta' \| \leq \frac{1}{2} L(\beta_{i'}) \right\}.$$

Thus, the factor $\lambda_{i'}$ which was derived in association with the vector $\beta_{i'}$ is weighted depending on the nearness of β' to $\beta_{i'}$.

III. RECOMMENDATIONS

The contractor recommends that the computation technique outlined above be utilized as soon as feasible in constructing least squares approximating functions of several variables. It is further recommended that this study be continued to include such items as:

1) The development of criteria for optimum data point selection.

2) The derivation of error bounds for least squares approximation models.

3) Extension of work in the selection of the best least squares approximating function.

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